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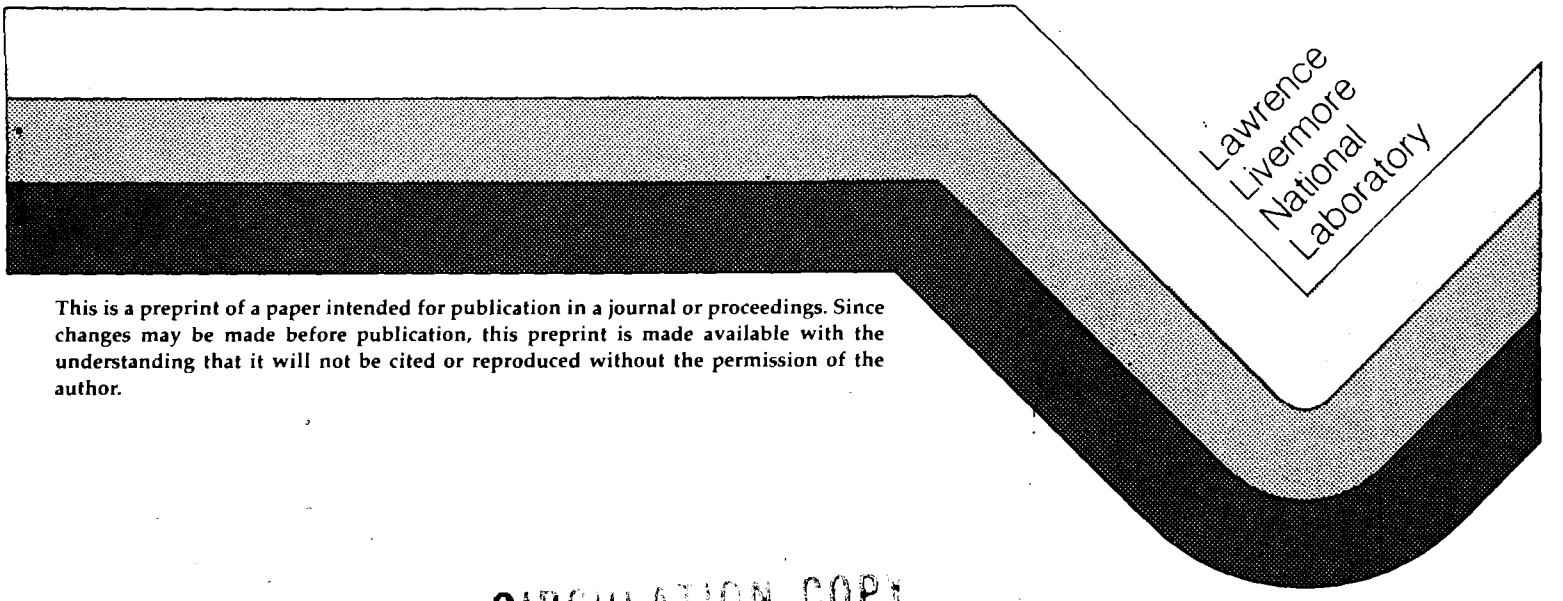

REMAPPING ON THE STAGGERED MESH

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ABSTRACT

The staggered mesh of von Neumann and Richtmyer provides a natural pattern of data storage for Lagrangian fluid dynamics. However, the solution of the advection equation, a necessary step for continuous rezone codes, leads to problems for fields stored on the nodes of the mesh, and in particular for the material velocities. In this paper, we describe a new scheme for advecting nodal quantities that is exactly conservative, computationally efficient and consistent in the sense of truncation error with the advection of cell-centered quantities.

INTRODUCTION

The staggered mesh scheme for computational fluid dynamics was first proposed by von Neumann and Richtmyer[1] and is still in common use today. On the staggered mesh the thermodynamic variables such as mass density, pressure and specific internal energy are stored at the centers of the computational cells whereas the dynamical variables such as material velocities are stored at the nodes. This storage pattern leads to a tight and efficient coupling between the fields for numerical solution of the equations of motion in a Lagrangian frame -- i.e., where the nodes are assumed to move with the local fluid velocity.

In principle the motion of the mesh can be chosen independently of the motion of the fluid. Continuous rezone or ALE (for Arbitrary Lagrangian-Eulerian) codes such as SHALE[2] exploit this independence. The aim is to reduce the mesh tangling associated with multidimensional Lagrangian calculations, and also to allow a degree of adaptivity of the mesh so that it better represent the fluid solution in regions of steep gradients. The hydrodynamics cycle in SHALE is broken into three separate phases. In the first phase, SHALE calculates a full Lagrangian update of the equations of motion over the computational cycle. In the second phase, SHALE determines a mesh motion with respect to the fluid based on some predetermined strategy. In the third phase, the Lagrangian solution is remapped onto the new mesh. This remapping procedure is often termed advection.

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The advection phase is really mathematical interpolation and is independent of the equations of motion. However, the advection algorithm is usually based on the physical idea of conservation. The advection of a cell-centered quantity in SHALE is conceptually straightforward. We restrict the motion of the mesh on any cycle so that the rezoned mesh is nearly the same as the Lagrangian mesh. (This means that we impose a Courant-like condition on the rezone velocities.) If we superpose the two meshes, then each cell in the new (rezoned) mesh coincides mainly with one cell of the old (Lagrangian) mesh. In addition the new cell may contain small volumes that were part of the nearest neighbors of the corresponding Lagrangian cell. Under these circumstances, we see the new mesh as being formed by the exchange of small pieces of volume between the cells of the old mesh. If we can assign a mass density to each small exchange volume, then we can ensure that each small increment of mass gained by a cell is exactly that lost by another. That is, we can enforce exact conservation. The various ways to choose the value of mass density in the exchange volume lead to the many different algorithms for advection that are now available.

In this paper, we shall simply assume that we have chosen some satisfactory scheme for cell-centered advection. Our concern focuses on another problem, remapping the nodal variables. There are at least three properties that a scheme for advecting nodal quantities should possess. These properties are accuracy, conservation and computational efficiency. These are the same general properties that we want our scheme for cell-centered advection to possess, and indeed the two schemes should be related. As an example, for consistency we would like the nodal advection to have the same accuracy as the cell-centered scheme, at least in the sense of truncation analysis. Also, most of the computational effort associated with cell-centered advection lies in the calculation of the overlap of the new and the old meshes and the exchange volumes. The nodal advection would be computationally most efficient if it used these same geometric terms.

Three schemes for advecting nodal quantities have been tried in the family of ALE-codes including YAQUI[3], SALE[4], and SHALE.[2] These schemes are

1. advection on the staggered mesh -- The method used in YAQUI is to create a second mesh such that the nodes of the first mesh are the cell centers of the second mesh. The idea of overlaying the grids and exchange volumes is repeated exactly on the second mesh.

2. advection of averaged quantities -- The method used in SALE is to average the nodal fields to create new variables at the cell centers. The variables are then advected like all other cell centered variables. The changes (n.b.) in these cell-centered variables are then redistributed back to the nodes.
3. interpolation -- Here we mean simple interpolation, independent of the overlay of the meshes. This scheme will not be exactly conservative.

Interpolation was tried in SHALE and discarded. It satisfies none of the three desirable properties listed above. In calculations, it is noisy in the sense of producing oscillations. Also, a strong shock can propagate with the wrong speed and the post - shock values of the thermodynamic quantities can have noticeable errors.

The YAQUI method is exactly conservative. However it requires calcuation of the exchange volumes on the second mesh and nearly doubles the CPU requirements. Its error is not quite consistent with the cell-centered scheme, because the rezone velocities must be averaged from the nodes to the cell centers to form the exchange volumes.

The SALE method is exactly conservative. It is also computationally efficient since all quantities are advected on the same mesh. However the redistribution process leads to a significant truncation error above that of cell-centered quantities. In practical terms, the SALE method also leads to large oscillations in regions of steep gradients. For very strong shocks, we found mesh waves created that dominated the physical aspects of the problem. Benson[5] has made a more detailed comparison of the YAQUI and SALE methods, with similar conclusions. He also shows that it is the redistribution process, rather than the underlying advection scheme, that causes the oscillations to appear.

In spite of its drawbacks, the SALE approach is closest to satisfying our three requirements. Our original idea was to improve the redistribution algorithm, which seems to be the weak point of the method, and this is effectively what we have done. However, it is easier to describe our new method from another point of view. In the next section, we will make some general comments about the advection operator. Then we will motivate our method for one-dimensional problems. We will next generalize our method for multi-dimensional problems on irregular meshes. Finally we will describe a simple modification that helps to further reduce oscillations in the advected fields.

THE TRANSLATION OPERATOR

The advection calculation is really an interpolation process necessitated by the rezoning of the mesh. The repositioning of the nodes of the cell changes the position of the cell center by δs. In operator notation and in one dimension, we write

$$(1) \qquad \Psi^{*}(x) = \mathbf{T}[\Psi(x)] = \Psi(x+\delta s)$$

where **T** is the translation operator. Using Taylor expansion, the continuum operator is

$$(2) \qquad \mathbf{T}[\Psi] = \Psi(x) + \frac{\partial \Psi}{\partial x}\delta s + \frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2}\delta s^2 + \ldots$$

The discrete approximation to the translation operator is defined by the advection algorithm, and so is nonunique. However, for any choice of algorithm, one can Taylor expand the discrete field. The numerical operator, $\mathbf{T}_\Delta$, in expanded form has the same form as Eq. (2). For consistency, the continuum operator and the discrete operator must agree for all terms up to order δs. For example, the expanded form of donor cell or upstream advection is

$$(3) \qquad \mathbf{T}_\Delta[\Psi] = \Psi(x) + \frac{\partial \Psi}{\partial x}\delta s + \frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2}\delta s\,\Delta x + \ldots$$

This agrees with Eq. (2) in its first two terms. The coefficient of the second order term agrees only when the displacement of the cell center, δs, equals the size of a cell, Δx. In fact, this is the situation where we are translating the entire profile one cell per time step. For a constant velocity field on a uniform mesh, it is possible to preserve exactly any profile using donor cell advection and a Courant number of 1. More generally we write

$$(4) \qquad \mathbf{T}_\Delta[\Psi] = \Psi(x) + \frac{\partial \Psi}{\partial x}\delta s + O\left(\frac{\partial^2 \Psi}{\partial x^2}\right) + \ldots$$

where the last term means of the order of the second derivative. The difference between Eq. (2) and Eq. (4) represents the truncation error.

For purposes of analyzing an advection scheme, it is necessary to specify the details of the numerical operator. However in this paper, we are concerned with the relationship between schemes for cell-centered and nodal advection. This relationship can be explored independently of the details of the particular underlying schemes. We will now use the same symbol **T** to denote the translation operator for the continuum and the discrete case, and rely on its argument to distinguish which one is used if this is important. We can write the SALE method in terms of this operator. In this method, we first construct the cell-centered average quantities

$$(5) \qquad A_{i+1/2} = \frac{1}{2}(\Psi_i + \Psi_{i+1}) = \text{Average}$$

Recall also that in the SALE method we redistribute the change in the advected quantity, and that the change corresponds to the operator **T-1.** The method is then written

$$(6) \qquad \Psi_i^{\cdot} = \Psi_i + \frac{1}{2}\left[[\mathbf{T}\text{-}1](A_{i+1/2}) + [\mathbf{T}\text{-}1](A_{i-1/2}) \right]$$

A ONE-DIMENSIONAL MODEL

The numerical operator is only defined for quantities defined at the cell centers. To apply this operator to quantities defined at the nodes, an obvious step is to represent the nodal quantities (at integral values of the logical variable i) in terms of cell-centered quantities (at half integral values of the logical variable i). For example, in one dimension on a constant mesh we define an additional cell-centered quantity

$$(7) \qquad D_{i+1/2} = (\Psi_{i+1} - \Psi_i) = \text{Difference}$$

The nodal field Ψ can be inverted in terms of the two cell-centered variables D and A

$$(8) \qquad \Psi_i = A_{i+1/2} - \frac{1}{2} D_{i+1/2}$$

The translation operator for the nodal quantity then can be defined by

$$(9) \qquad \mathbf{T}[\Psi_i] \equiv \mathbf{T}\left[A_{i+1/2}\right] - \frac{1}{2}\mathbf{T}\left[D_{i+1/2}\right]$$

The right hand side of Eq. (7) is perfectly well-defined. The representation

$$(10) \qquad \Psi_i = A_{i-1/2} + \frac{1}{2} D_{i-1/2}$$

would be an equally valid, though distinct way to represent the nodal quantity.

If we expanded Eq. (8) about the cell center and then applied the operator defined in Eq. (9), we would find the right-hand-side contains one extra term beyond the truncation error of the cell-centered variables. The origin of this term can be traced to the lack of symmetry of the representation in Eq. (8), and can be removed by using an average of the representations of Eqs. (8) and (10). For fluid flow problems, it is also advantageous to redistribute the change in the advected variables, for reasons having to do with vertex mass. Thus, in one dimension on a uniform mesh, we would define our nodal advection

$$(11) \qquad \begin{aligned} \Psi_i^* = \mathbf{T}[\Psi_i] \equiv \Psi_i &+ \frac{1}{2}[\mathbf{T}\text{-}1]\left[A_{i+1/2}\right] - \frac{1}{4}[\mathbf{T}\text{-}1]\left[D_{i+1/2}\right] \\ &+ \frac{1}{2}[\mathbf{T}\text{-}1]\left[A_{i-1/2}\right] + \frac{1}{4}[\mathbf{T}\text{-}1]\left[D_{i-1/2}\right] \end{aligned}$$

In words, Eq. (11) says:

1. form two sets of cell-centered quantities, the average and the difference of the nodal fields;
2. advect both these fields using the cell-centered advection scheme;
3. distribute half the change in the average field to each node. Add one quarter of the change in the difference field to the node on the left and subtract it from the node on the right.

The last point can be interpreted as being a more accurate method of redistributing the changes of the advected field. The additional accuracy is the result of having more information -- i.e., the information contained in the second advected field.

The relationship between the Ψ field and the A and D fields seems to imply a simple change of basis functions. This is not quite correct, for there are twice as many elements in the set {A,D} as in the set {Ψ}. In principle, the set {D} is extraneous, and the changes in the nodal fields could be found by inverting Eq. (4), written for the advected fields, with appropriate boundary conditions. However, this would require inverting a mesh-sized array. One way to view the use of the set {D} is that it allows us to find an approximate, but explicit solution to the implicit problem of redistributing the changes in the advected field from the cell centers to the nodes.

IRREGULAR MULTIDIMENSIONAL MESHES

The extension of Eq. (11) to irregularly shaped cells in two- and three-dimensional calculations is simple. The average fields are defined in eactly the same way . For example, in two dimensions we write

$$(12) \qquad \widehat{\Psi}_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{1}{4}\left[\Psi_{i,j} + \Psi_{i+1,j} + \Psi_{i,j+1} + \Psi_{i+1,j+1}\right]$$

We replace the difference fields by the spatial derivatives. Recalling that in two and three dimensions, the nodal fields are velocities and hence vectors, there are four derivatives in two dimensions and nine in three dimensions --

$$\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \ldots$$

The necessary steps for advecting the nodal velocities in two dimensions are:

1. form the six cell-centered quantities, which are the average Ψ and the average φ, and the four derivatives;
2. advect each of these using the cell-centered algorithm;
3. redistribute the changes in each of the six variables using a Taylor series expansion.

The algorithm is written explicitly as

$$\Psi^{*}_{i,j} = T[\Psi_{i,j}] \equiv \Psi_{i,j} + \frac{1}{4}[T-1]\left[\widehat{\Psi}_{i+1/2,j+1/2}\right]$$

$$+ \frac{1}{4}[T-1]\left[\left[\frac{\partial\Psi}{\partial x}\right]_{i+1/2,j+1/2}\right](x^{*}_{i,j} - x^{*}_{i+1/2,j+1/2}) \tag{13}$$

$$+ \frac{1}{4}[T-1]\left[\left[\frac{\partial\Psi}{\partial y}\right]_{i+1/2,j+1/2}\right](y^{*}_{i,j} - y^{*}_{i+1/2,j+1/2})$$

$$+ \text{terms in } (i\text{-}1/2,j\text{+}1/2), (i\text{+}1/2,j\text{-}1/2) \text{ and } (i\text{-}1/2,j\text{-}1/2)$$

Note that in Eq. (13), the rezoned coordinates (x^{*}, y^{*}) are used in the Taylor series.

FURTHER MODIFICATIONS

One further modification has been found to improve the performance of our nodal advection scheme, in the sense of reducing spurious oscillations. Benson[5] notes that in the schemes he investigated, monotonicity of the algorithm for cell-centered variables does not guarantee monotonicity for nodal variables. We have found the same result for our new scheme. A heuristic analysis (which we do not present here) suggests that many of these oscillations would be eliminated if we used a donor cell scheme to advect the derivatives whatever cell-centered scheme is used. Since the difference between the various advection schemes is of the order of the second derivative, and these are applied to a term that is already of the order of the first derivative, this change is seen only in the higher order terms of the truncation analysis.

SUMMARY

We have developed a new scheme for advecting nodal quantities. The scheme is exactly conservative. It is consistent with the cell-centered advection scheme in the sense that it has the same truncation error. The scheme is computationally efficient in that it depends on advecting extra cell-centered variables, and requires only minimal additional goemetric calculations.

The basic idea is an extension of the SALE method, which constructs new cell-centered fields that are average values of the nodal fields, and advects these averaged fields. In SALE, the changes in the averaged fields are redistributed equally back to the nodes. Our new scheme constructs several extra fields, which are spatial derivatives of the nodal fields and advects these in addition. The changes in the advected derivatives are then used for a more accurate redistribution of the changes in the average fields, based on a Taylor series expansion. Equation (13) describes the process in mathematical detail.

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